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title: "Re-walk the path of Niels Bohr"

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I feel rather like Bohr, when calculating the Lennard Jones potential. Bohr had to put up with an orbital theory with quantized energy levels, in order to explain the atomic reflection spectra. Here we had to approximate the atomic interactions, reduce the form of equations and then what, "cutoff" the tail and assume a finite repeating unit? I thought we have immense power witht the modern computers.

**It is probably easy thought than done**

Lennard Jones used more than 30 pages and 50 deductions to come up with an approximation, that to any scientist of theoretical chemistry can perfectly fit gas interaction within a braod range of temperatures. In addition, it fits rather well with predict how atomic

# Cutoffs

Consider a system of 10 particles. How many pairwise particle-particle interactions will there be? What about 100 or 1000 particles? Consider a system with a density of 1. Using this density, how many particles are in a sphere with radius 1, 2, 5, and 10 units? (These are math problems, you don’t have to use programming to solve them, but you can.)

The general format of pairwise particle interactions for n particles is:

n \* (n-1) / 2

For 10 particles: 45 interactions.

For 100 particles: 4950 interactions.

For 1000 particles: 499500 interactions.

The volume of a sphere with radius r is 4/3 \* pi \* (r \*\* 3).

With unit density of 1, the number of particles within the sphere volume is [4/3 \* pi \* (r \*\* 3) // 1]

Can you think of the benefits associated with using a cut-off? What are the risks?

The benefits are: Reduce the cost of computation. Save time of effort.

The risks are: The method is less accurate. It might affect the final result.

# Periodic Boundaries

Consider the following questions:

What is the maximum distance any particle can be from another in each dimension? (this will have to do with the box length)

Given periodic boundary, and assume that all boxes are identical and are smallest repeating units, the max distance in each dimension is (Box-length / 2)

What is the actual distance of our example? ((0, 0, 0), (0, 0, 8))

Given a Box-length of 10, the actual distance between the two particles is (Box-length - 8) = 2.